

Adipic acid, isohexyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C25H32O5/c1-20(2)10-9-17-28-24(26)15-6-7-16-25(27)29-19-21-11-8-14-23(1
InchiKey:	VLOXDVLDLWWVRQ-UHFFFAOYSA-N
Formula:	C25H32O5
SMILES:	CC(C)CCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	412.52

Physical Properties

Property code	Value	Unit	Source
gf	-200.47	kJ/mol	Joback Method
hf	-724.84	kJ/mol	Joback Method
hfus	51.44	kJ/mol	Joback Method
hvap	96.79	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.062		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinsol	3045.00		NIST Webbook
tb	1004.30	K	Joback Method
tc	1232.41	K	Joback Method
tf	588.42	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.72	J/molxK	1004.30	Joback Method
cpg	1118.21	J/molxK	1042.32	Joback Method
cpg	1130.08	J/molxK	1080.34	Joback Method
cpg	1140.37	J/molxK	1118.36	Joback Method
cpg	1149.13	J/molxK	1156.38	Joback Method
cpg	1156.41	J/molxK	1194.39	Joback Method
cpg	1162.23	J/molxK	1232.41	Joback Method
dvisc	0.0002284	Paxs	588.42	Joback Method
dvisc	0.0001204	Paxs	657.73	Joback Method

dvisc	0.0000717	Paxs	727.05	Joback Method
dvisc	0.0000467	Paxs	796.36	Joback Method
dvisc	0.0000326	Paxs	865.67	Joback Method
dvisc	0.0000240	Paxs	934.99	Joback Method
dvisc	0.0000184	Paxs	1004.30	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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